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Brownian dynamics simulation of polymer chains incorporating bending and torsion potentials SEMANT JAIN, RONALD LARSON, University of Michigan — Using stretching, bending, and torsion potentials for linear alkanes as described in literature [Ryckaet and Bellemans (1975), Helfand et al. (1980)], we study polymer state transitions, coil size, and storage and loss modulii. As the chain size increases, we compare the coil expansion resulting from bending and torsion forces to the theoretical predictions. Additionally, we compare the effect of Helfand's stretching and bending parameters, commonly used to speed up computation, versus realistic parameters in predicting the impact on coil size. Finally, we vary barrier heights between gauche+/- and trans torsional transition states to identify the limiting factor between bond orientation transitions. We compute individual bond vector and end-to-end vector correlations by combining Brownian force with spring, bending, and torsion forces to predict the contribution of each to the spectrum of polymer relaxation times.

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